



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:36 PM GMT

PDB ID : 1UES  
Title : Crystal structure of Porphyromonas gingivalis SOD  
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Deposited on : 2003-05-20  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

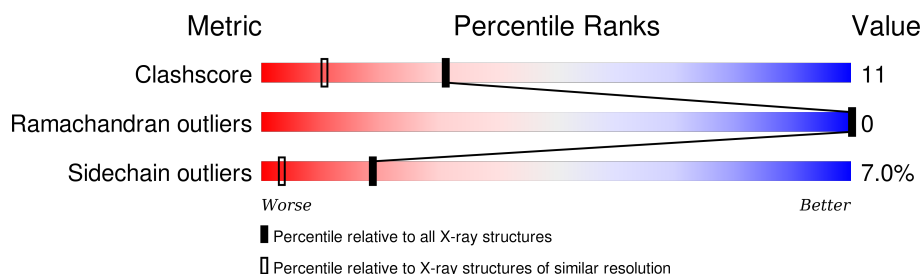
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	191	
1	B	191	
1	C	191	
1	D	191	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6472 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1529	982	259	287	1			
1	B	191	Total	C	N	O	S	0	0	0
			1529	982	259	287	1			
1	C	191	Total	C	N	O	S	0	0	0
			1529	982	259	287	1			
1	D	191	Total	C	N	O	S	0	0	0
			1529	982	259	287	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	THR	GLY	ENGINEERED	UNP P19665
B	355	THR	GLY	ENGINEERED	UNP P19665
C	555	THR	GLY	ENGINEERED	UNP P19665
D	755	THR	GLY	ENGINEERED	UNP P19665

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is water.

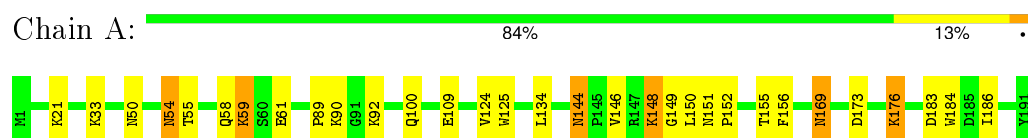
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total 124	O 124	0	0
3	B	60	Total 60	O 60	0	0
3	C	72	Total 72	O 72	0	0
3	D	96	Total 96	O 96	0	0

### 3 Residue-property plots

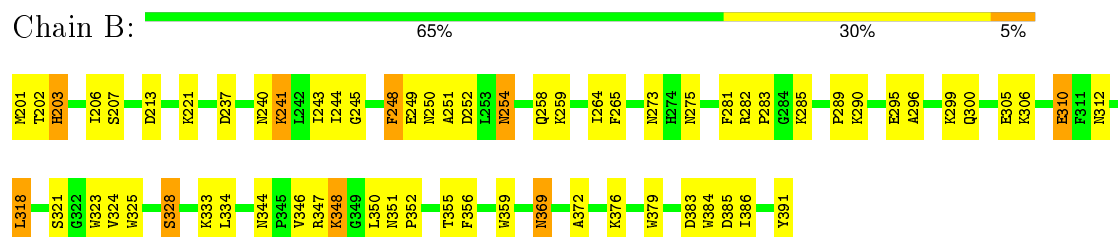
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

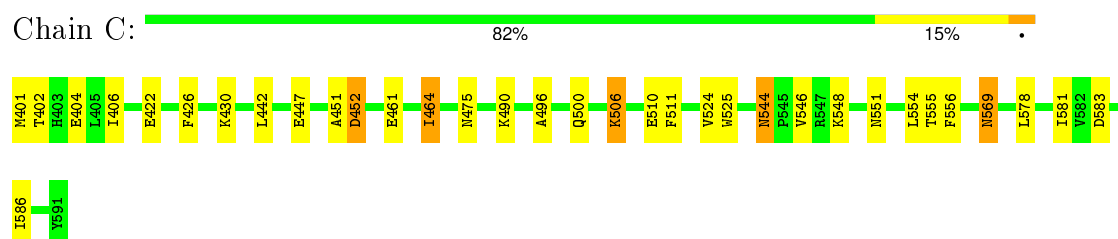
- Molecule 1: superoxide dismutase



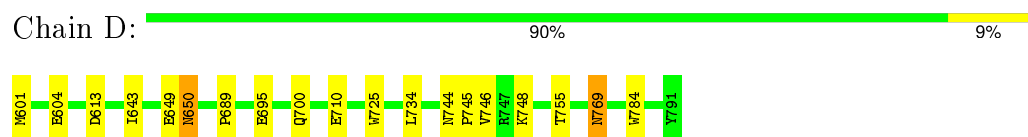
- Molecule 1: superoxide dismutase



- Molecule 1: superoxide dismutase



- Molecule 1: superoxide dismutase



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.68Å 95.12Å 98.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.60)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, $R_{free}$	0.221 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.56	0/1570	0.72	0/2127
1	B	0.47	0/1570	0.68	0/2127
1	C	0.45	0/1570	0.64	0/2127
1	D	0.49	0/1570	0.70	0/2127
All	All	0.50	0/6280	0.69	0/8508

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1529	0	1483	29	0
1	B	1529	0	1480	56	0
1	C	1529	0	1480	28	0
1	D	1529	0	1480	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	124	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	60	0	0	2	0
3	C	72	0	0	2	0
3	D	96	0	0	2	0
All	All	6472	0	5923	130	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:601:MET:HE3	1:D:650:ASN:HB3	1.35	1.07
1:A:146:VAL:HA	3:A:301:HOH:O	1.62	1.00
1:A:100:GLN:HE22	1:A:134:LEU:H	1.07	0.97
1:A:173:ASP:HA	1:A:176:LYS:HD3	1.50	0.92
1:D:700:GLN:NE2	1:D:734:LEU:H	1.68	0.89
1:D:700:GLN:HE22	1:D:734:LEU:H	0.94	0.89
1:B:300:GLN:HE22	1:B:334:LEU:H	1.20	0.86
1:D:700:GLN:HE22	1:D:734:LEU:N	1.76	0.83
1:D:744:ASN:HD22	1:D:746:VAL:H	1.24	0.82
1:B:306:LYS:O	1:B:310:GLU:HG2	1.79	0.82
1:D:601:MET:CE	1:D:650:ASN:HB3	2.09	0.82
1:C:524:VAL:HG12	1:C:556:PHE:HB2	1.65	0.78
1:D:643:ILE:HD13	1:D:649:GLU:HA	1.65	0.78
1:B:264:ILE:HD12	1:B:264:ILE:H	1.50	0.77
1:C:544:ASN:HD22	1:C:546:VAL:H	1.32	0.76
1:B:312:ASN:HD21	1:B:379:TRP:HE1	1.32	0.76
1:A:144:ASN:HD22	1:A:146:VAL:H	1.33	0.74
1:B:344:ASN:ND2	1:B:346:VAL:H	1.84	0.74
1:A:54:ASN:O	1:A:58:GLN:HG3	1.88	0.74
1:B:296:ALA:O	1:B:300:GLN:HG3	1.87	0.74
1:A:144:ASN:HD21	1:A:146:VAL:HG13	1.51	0.73
1:D:601:MET:HE3	1:D:650:ASN:CB	2.16	0.73
1:A:144:ASN:ND2	1:A:146:VAL:HG13	2.04	0.73
1:B:344:ASN:HD22	1:B:346:VAL:H	1.40	0.70
1:A:169:ASN:HD22	1:A:169:ASN:H	1.39	0.69
1:C:464:ILE:HD13	3:C:213:HOH:O	1.92	0.69
1:A:151:ASN:HB2	3:A:243:HOH:O	1.93	0.68
1:B:283:PRO:HA	3:B:416:HOH:O	1.94	0.68
1:B:241:LYS:HD3	1:B:241:LYS:N	2.09	0.68
1:B:295:GLU:O	1:B:299:LYS:HD3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:NE2	1:A:134:LEU:H	1.86	0.67
1:C:524:VAL:CG1	1:C:556:PHE:HB2	2.25	0.66
1:D:744:ASN:ND2	1:D:746:VAL:H	1.95	0.65
1:D:769:ASN:HD22	1:D:769:ASN:H	1.45	0.65
1:A:144:ASN:ND2	1:A:146:VAL:H	1.95	0.64
1:C:496:ALA:O	1:C:500:GLN:HG3	1.98	0.64
1:B:254:ASN:O	1:B:258:GLN:HG2	1.98	0.64
1:C:464:ILE:CD1	1:C:464:ILE:N	2.61	0.64
1:C:401:MET:HG2	1:C:401:MET:O	1.99	0.62
1:C:506:LYS:O	1:C:506:LYS:HE2	1.99	0.62
1:B:300:GLN:HB3	3:B:402:HOH:O	1.99	0.62
1:B:383:ASP:HB3	1:B:386:ILE:HD12	1.84	0.60
1:B:203:HIS:H	1:B:203:HIS:CD2	2.20	0.59
1:B:300:GLN:NE2	1:B:334:LEU:H	1.97	0.58
1:A:21:LYS:HE3	3:A:298:HOH:O	2.03	0.58
1:C:442:LEU:HD13	1:C:464:ILE:HD12	1.86	0.58
1:B:265:PHE:CE1	1:B:347:ARG:HD2	2.40	0.57
1:C:544:ASN:ND2	1:C:546:VAL:H	2.02	0.56
1:B:203:HIS:CD2	1:B:203:HIS:N	2.74	0.56
1:B:206:ILE:HG12	1:B:275:ASN:OD1	2.06	0.55
1:D:643:ILE:CD1	1:D:649:GLU:HA	2.38	0.54
1:B:213:ASP:HB3	1:B:221:LYS:HD2	1.88	0.54
1:A:124:VAL:CG1	1:A:156:PHE:HB2	2.37	0.54
1:C:401:MET:CE	1:C:452:ASP:HA	2.38	0.54
1:D:725:TRP:CD2	1:D:755:THR:HB	2.43	0.54
1:A:21:LYS:HG2	3:A:300:HOH:O	2.08	0.54
1:C:464:ILE:H	1:C:464:ILE:HD13	1.74	0.53
1:C:422:GLU:H	1:C:422:GLU:CD	2.12	0.53
1:C:544:ASN:ND2	1:C:546:VAL:HG13	2.24	0.53
1:B:369:ASN:HD22	1:B:369:ASN:H	1.56	0.52
1:B:282:ARG:HB2	1:B:285:LYS:CG	2.40	0.52
1:B:325:TRP:CD2	1:B:355:THR:HB	2.44	0.52
1:B:282:ARG:HB2	1:B:285:LYS:HG3	1.91	0.52
1:A:173:ASP:HA	1:A:176:LYS:CD	2.31	0.52
1:B:324:VAL:CG1	1:B:356:PHE:HB2	2.40	0.52
1:C:426:PHE:CD1	1:C:430:LYS:HD2	2.45	0.52
1:D:604:GLU:HG2	3:D:352:HOH:O	2.08	0.51
1:C:544:ASN:HD21	1:C:546:VAL:HG13	1.75	0.51
1:A:125:TRP:CZ3	1:A:152:PRO:HB2	2.46	0.51
1:A:55:THR:HG23	1:A:59:LYS:HD2	1.94	0.50
1:C:525:TRP:CE3	1:C:555:THR:HB	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ASP:O	1:B:241:LYS:HD3	2.13	0.49
1:C:569:ASN:HD22	1:C:569:ASN:H	1.59	0.49
1:A:55:THR:CG2	1:A:59:LYS:HD2	2.43	0.49
1:C:506:LYS:HE2	1:C:510:GLU:HG3	1.94	0.48
1:A:151:ASN:CB	3:A:243:HOH:O	2.56	0.48
1:C:406:ILE:HG12	1:C:475:ASN:OD1	2.13	0.48
1:A:183:ASP:HB3	1:A:186:ILE:HD12	1.95	0.48
1:A:125:TRP:CD2	1:A:155:THR:HB	2.48	0.48
1:D:725:TRP:CE2	1:D:755:THR:HB	2.49	0.48
1:C:578:LEU:HD23	1:C:581:ILE:HD11	1.96	0.47
1:C:442:LEU:HB3	1:C:464:ILE:HD11	1.97	0.47
1:B:344:ASN:HD22	1:B:346:VAL:N	2.10	0.47
1:B:241:LYS:N	1:B:241:LYS:CD	2.78	0.47
1:A:169:ASN:H	1:A:169:ASN:ND2	2.10	0.47
1:B:325:TRP:CZ3	1:B:352:PRO:HB2	2.51	0.46
1:B:243:ILE:C	1:B:249:GLU:HG3	2.35	0.46
1:B:201:MET:O	1:B:243:ILE:HG21	2.15	0.46
1:B:201:MET:HB3	1:B:249:GLU:O	2.16	0.46
1:A:89:PRO:HB3	1:A:184:TRP:CE3	2.51	0.46
1:B:202:THR:HG22	1:B:202:THR:O	2.16	0.46
1:B:248:PHE:O	1:B:249:GLU:C	2.53	0.46
1:B:328:SER:HG	1:B:391:TYR:HE1	1.61	0.45
1:B:372:ALA:O	1:B:376:LYS:HG3	2.17	0.45
1:B:243:ILE:HD12	1:B:244:ILE:N	2.31	0.45
1:D:689:PRO:HB3	1:D:784:TRP:CE3	2.52	0.45
1:A:149:GLY:CA	3:A:301:HOH:O	2.64	0.44
1:B:321:SER:HB3	1:B:359:TRP:CD2	2.53	0.44
1:B:273:ASN:HB3	1:B:323:TRP:CZ2	2.52	0.44
1:C:401:MET:SD	1:C:451:ALA:O	2.75	0.44
1:B:201:MET:N	1:B:249:GLU:O	2.51	0.44
1:B:325:TRP:CE3	1:B:355:THR:HB	2.52	0.44
1:B:201:MET:HB2	1:B:250:ASN:HA	1.99	0.44
1:C:464:ILE:HD12	1:C:464:ILE:N	2.31	0.43
1:A:100:GLN:HE22	1:A:134:LEU:N	1.92	0.43
1:B:281:PHE:O	1:B:282:ARG:HG2	2.18	0.43
1:B:289:PRO:HB3	1:B:384:TRP:CE3	2.53	0.43
1:C:461:GLU:HB3	3:C:231:HOH:O	2.18	0.43
1:C:511:PHE:CE1	1:C:524:VAL:HG13	2.54	0.43
1:B:328:SER:OG	1:B:391:TYR:HE1	2.02	0.43
1:B:344:ASN:HD21	1:B:346:VAL:HG23	1.84	0.43
1:B:245:GLY:H	1:B:249:GLU:CD	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:MET:HG2	1:B:251:ALA:O	2.19	0.42
1:B:240:ASN:O	1:B:243:ILE:HG13	2.19	0.42
1:B:383:ASP:CB	1:B:386:ILE:HD12	2.50	0.42
1:B:249:GLU:HB3	1:B:250:ASN:HD22	1.84	0.42
1:B:348:LYS:HB2	1:B:350:LEU:HG	2.01	0.42
1:A:144:ASN:ND2	1:A:146:VAL:HG22	2.35	0.42
1:C:583:ASP:HB3	1:C:586:ILE:HD12	2.01	0.42
1:A:150:LEU:N	3:A:301:HOH:O	2.52	0.41
1:A:125:TRP:CE2	1:A:155:THR:HB	2.55	0.41
1:D:710:GLU:HG3	3:D:306:HOH:O	2.21	0.41
1:A:148:LYS:HB2	1:A:148:LYS:HE2	1.72	0.41
1:C:506:LYS:CE	1:C:510:GLU:HG3	2.50	0.41
1:B:318:LEU:C	1:B:318:LEU:HD12	2.40	0.41
1:B:201:MET:HB2	1:B:251:ALA:H	1.85	0.41
1:B:300:GLN:NE2	1:B:333:LYS:HD2	2.35	0.41
1:B:310:GLU:HG2	1:B:310:GLU:H	1.67	0.41
1:B:312:ASN:ND2	1:B:379:TRP:HE1	2.09	0.41
1:D:744:ASN:HA	1:D:745:PRO:HD3	1.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	189/191 (99%)	184 (97%)	5 (3%)	0	100	100
1	B	189/191 (99%)	181 (96%)	8 (4%)	0	100	100
1	C	189/191 (99%)	182 (96%)	7 (4%)	0	100	100
1	D	189/191 (99%)	184 (97%)	5 (3%)	0	100	100
All	All	756/764 (99%)	731 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	161/161 (100%)	149 (92%)	12 (8%)	17	3
1	B	161/161 (100%)	145 (90%)	16 (10%)	10	1
1	C	161/161 (100%)	149 (92%)	12 (8%)	17	3
1	D	161/161 (100%)	156 (97%)	5 (3%)	47	19
All	All	644/644 (100%)	599 (93%)	45 (7%)	19	3

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	50	ASN
1	A	54	ASN
1	A	59	LYS
1	A	61	GLU
1	A	90	LYS
1	A	92	LYS
1	A	109	GLU
1	A	144	ASN
1	A	148	LYS
1	A	169	ASN
1	A	176	LYS
1	B	203	HIS
1	B	207	SER
1	B	241	LYS
1	B	248	PHE
1	B	252	ASP
1	B	254	ASN
1	B	259	LYS
1	B	290	LYS
1	B	305	GLU
1	B	310	GLU
1	B	318	LEU
1	B	328	SER

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Mol	Chain	Res	Type
1	B	348	LYS
1	B	351	ASN
1	B	369	ASN
1	B	385	ASP
1	C	402	THR
1	C	404	GLU
1	C	447	GLU
1	C	452	ASP
1	C	464	ILE
1	C	490	LYS
1	C	506	LYS
1	C	544	ASN
1	C	548	LYS
1	C	551	ASN
1	C	554	LEU
1	C	569	ASN
1	D	613	ASP
1	D	650	ASN
1	D	695	GLU
1	D	748	LYS
1	D	769	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	144	ASN
1	A	169	ASN
1	B	203	HIS
1	B	250	ASN
1	B	300	GLN
1	B	312	ASN
1	B	344	ASN
1	B	369	ASN
1	C	454	ASN
1	C	458	GLN
1	C	544	ASN
1	C	569	ASN
1	D	700	GLN
1	D	744	ASN
1	D	769	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.